X-ray Absorption Spectroscopy of Alkanes – Old Mysteries, New Questions

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The C 1s Near Edge X-ray Absorption Fine Structure (NEXAFS) spectra of alkanes are complex and are a long standing matter of controversy. Alkanes are a class of saturated molecules that range from simple hydrocarbons such as methane to macromolecules such as polyethylene. The gas and solid phase spectra of alkanes are remarkably different, indicating the complex role of “matrix effects” in their spectra. While the linear dichroism in their NEXAFS spectra is frequently used for measuring molecular orientation in self-assembled monolayers, there is no consensus for the underlying spectroscopic description of this effect. This talk will address our efforts to address these interrelated questions through a combined program of experiment and computational studies, as well as recent efforts to study the nanoscale orientation in thin films of alkanes, their dynamics, and the development of methods to control and define molecular orientation in these materials.